

# Subextensive singularity in the 2D $\pm J$ Ising spin glass

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## Abstract

The statistics of low energy states of the 2D Ising spin glass with +1 and -1 bonds are studied for  $L \times L$  square lattices with  $L \leq 48$ , and  $p = 0.5$ , where  $p$  is the fraction of negative bonds, using periodic and/or antiperiodic boundary conditions. The behavior of the density of states near the ground state energy is analyzed as a function of  $L$ , in order to obtain the low temperature behavior of the model. For large finite  $L$  there is a range of  $T$  in which the heat capacity is proportional to  $T^{5.33 \pm 0.12}$ . The range of  $T$  in which this behavior occurs scales slowly to  $T = 0$  as  $L$  increases. Similar results are found for  $p = 0.25$ . Our results indicate that this model probably obeys the ordinary hyperscaling relation  $d\nu = 2 - \alpha$ , even though  $T_c = 0$ . The existence of the subextensive behavior is attributed to long-range correlations between zero-energy domain walls, and evidence of such correlations is presented.

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In 1977, Thouless, Anderson and Palmer<sup>1</sup> (TAP) performed a mean-field theory analysis of the ring diagrams which contribute to the free energy of the Ising spin glass.<sup>2,3</sup> They found that, above the critical temperature  $T_g$ , the contribution of these ring diagrams was subextensive. This means that, while the sum of these diagrams is divergent at  $T_g$ , their contribution at any  $T > T_g$  can be neglected in the thermodynamic limit.<sup>3</sup> Therefore, in this limit, no signature of the transition is visible in the equilibrium thermodynamic functions for  $T > T_g$ . However, one can still study the critical scaling behavior of finite systems.

While it is true that hyperscaling is always violated in a mean-field theory, TAP showed that a spin glass has severe fluctuations of the order parameter even at the mean-field level. Later, it was shown by Sompolinsky and Zippelius<sup>4,5</sup> that the Ising spin glass also violates the fluctuation-dissipation theorem. Thus one should not be surprised if it turns out that the spin glass does not obey other relations which work for ordinary phase transitions.

In this work we analyze data obtained from exact calculations of the density of low-energy states for finite two-dimensional (2D) lattices. The same data have also been used to study the scaling behavior of domain walls for this model.<sup>6</sup> We will discover that an unusual effect, similar to the violation of hyperscaling found in mean-field theory, also occurs in 2D. The data were obtained using a slightly modified version of the computer program of Vondrák,<sup>7,8</sup> which is based on the Pfaffian method. Our data are completely consistent with the data of Lukic *et al.*,<sup>10,11</sup> which were obtained using the same algorithm. Our analysis of the heat capacity is more detailed than theirs, however, and thus we arrive at somewhat different conclusions.

In two dimensions (2D), the spin-glass phase is not stable at finite temperature. Because of this, it is necessary to treat cases with continuous distributions of energies (CDE) and cases with quantized distributions of energies (QDE) separately.<sup>12,13</sup> In this work we will study the QDE case.

The Hamiltonian of the EA model for Ising spins<sup>2</sup> is

$$H = - \sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j, \quad (1)$$

where each spin  $\sigma_i$  is a dynamical variable which has two allowed states, +1 and -1. The  $\langle ij \rangle$  indicates a sum over nearest neighbors on a simple square lattice of size  $L \times L$ . We choose each bond  $J_{ij}$  to be an independent identically distributed quenched random variable, with

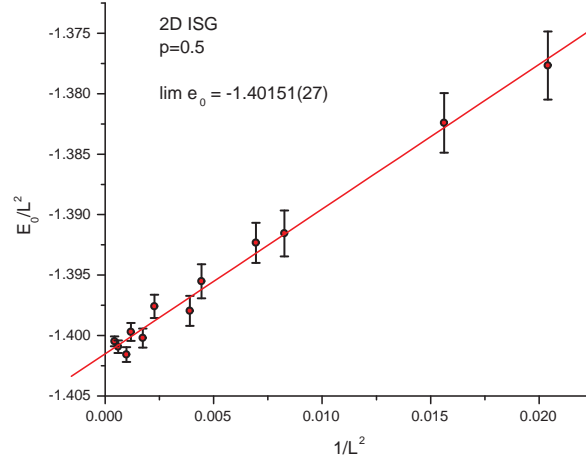


FIG. 1: (color online) Finite-size scaling of  $E_0/L^2$  vs.  $1/L^2$ .

the probability distribution

$$P(J_{ij}) = p\delta(J_{ij} + 1) + (1 - p)\delta(J_{ij} - 1), \quad (2)$$

so that we actually set  $J = 1$ , as usual. Thus  $p$  is the concentration of antiferromagnetic bonds, and  $(1 - p)$  is the concentration of ferromagnetic bonds. Here we will discuss primarily the equal mixture case,  $p = 0.5$ , but results for  $p = 0.25$  will also be given.

The ground state (GS) entropy is defined as the natural logarithm of the number of ground states. For each sample the GS energy  $E_0$  and GS entropy  $S_0$  were calculated for the four combinations of periodic and antiperiodic toroidal boundary conditions along each of the two axes of the square lattice. When  $p = 0.5$ , all four of these types of boundary conditions are statistically equivalent.

Data were obtained for lattices of sizes  $L = 7, 8, 11, 12, 15, 16, 21, 24, 29, 32, 41$  and  $48$ . For each  $L$ , 500 different random sets of bonds were studied, for each of the four boundary conditions. Thus, combining the data for the different boundary conditions, we have 2000 values of  $E_0$  and  $S_0$  for each  $L$ .

With the boundary conditions we are using, for which there is no well-defined surface, the value of  $E_0$  averaged over samples of the random bonds, is expected to obey

$$E_0/L^2 = e_0 + a_e/L^2 \quad (3)$$

to lowest order in  $L$ . Fig. 1 shows that this works well, and that the value of  $e_0$  obtained from our data is  $e_0 = -1.40151 \pm 0.00027$ . In principle, higher order corrections exist,<sup>9</sup> but

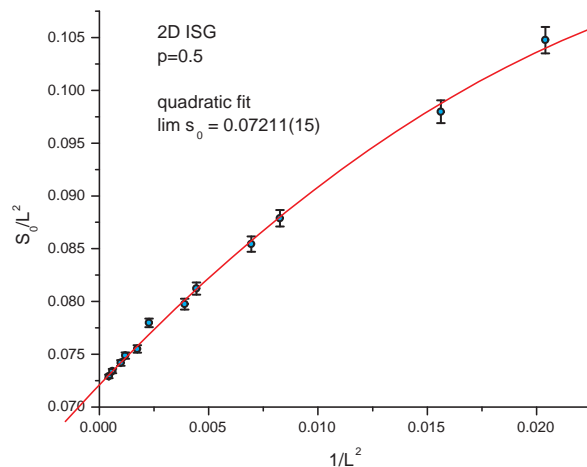


FIG. 2: (color online) Finite-size scaling of  $S_0/L^2$  vs.  $1/L^2$ .

they are not necessary at the level of precision of our data. This agrees with the result found by Lukic *et al.*<sup>10</sup> All statistical error estimates shown in this work represent one standard deviation. The best estimate of  $e_0$  is still the one of Palmer and Adler,<sup>14</sup> which uses a method for which one can go to much larger  $L$ , because the entropy is not calculated.

The finite-size scaling behavior of  $S_0$  is slightly more complex. Lukic *et al.*<sup>10</sup> used a single correction-to-scaling term, with an exponent  $-(2 + \Theta_S)$ . From a fundamental viewpoint,<sup>15</sup> however, when  $\Theta_S$  is positive the natural form to use when adding another fitting parameter is

$$S_0/L^2 = s_0 + a_s/L^2 + b_s/L^4. \quad (4)$$

In Fig. 2 we see that this form works well, and gives a value of  $s_0 = 0.07211 \pm 0.00015$ . This value is slightly higher than the one quoted by Lukic *et al.*, but the difference comes primarily from the different form of the fitting function rather than from differences in the data. By comparing with the work of Bouchaud, Krzakala and Martin,<sup>15</sup> one sees that Lukic *et al.* have made a sign error, and that their fit actually uses a negative value for  $\Theta_S$ , which is incorrect.<sup>16,17</sup>

While our values of the energy and entropy of the GS of finite  $L \times L$  lattices for  $p = 0.5$  are generally consistent with those of other workers, our results for  $L = 32$  differ substantially with those reported by Blackman and Poulter.<sup>18</sup> (See Figs. 7 and 8 of their paper.) The origin of this discrepancy is unclear, but it appears to be too large to be explained by the

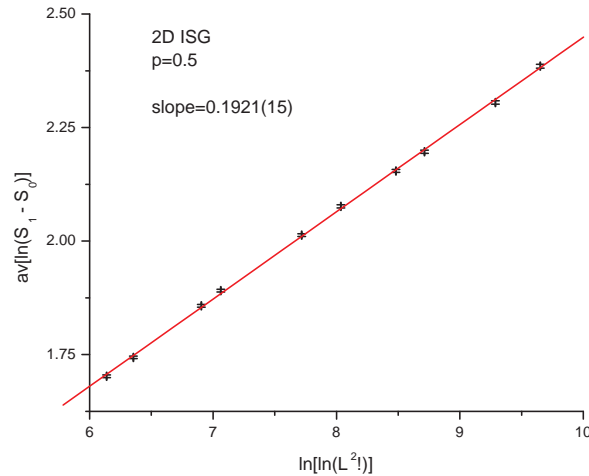


FIG. 3: (color online) Scaling of  $S_1 - S_0$  with  $L$ .

different boundary conditions used by them. Their numbers of samples computed are rather small, and it may be that they have simply underestimated their statistical errors. However, their algorithm, unlike the one used here, does not use exact integer arithmetic to calculate the partition function. Therefore, it is likely that they have a problem with roundoff errors. In a strongly correlated system such as the one we are studying, substantial roundoff errors can result in distributions which are too narrow.

In order to obtain information about the low temperature behavior, it is useful to study the scaling with  $L$  of  $S_1 - S_0$ , which is the logarithm of the ratio of the degeneracies of the lowest excited state and the GS.<sup>10,16,17,19</sup> We found that

$$\text{av}(\ln(S_1 - S_0)) = \rho \ln(\ln((L^2)!)) + 0.528 \pm 0.011, \quad (5)$$

with

$$\rho = 0.1921 \pm 0.0015 \quad (6)$$

gives an excellent fit for  $L > 10$ , as shown in Fig. 3.  $\text{av}()$  is a configuration average over random samples. The points for  $L = 7$  and  $8$  (not shown in the figure) are below the fitted line, due to corrections to scaling at small  $L$ .

The choice  $\ln(\ln((L^2)!))$  may appear arbitrary to the reader, but it was suggested by the behavior of the fully frustrated 2D Ising model.<sup>16,17</sup> In principle, if one could go to very large values of  $L$ , one could obtain  $\rho$  by plotting the data against  $2\ln(L)$ . From

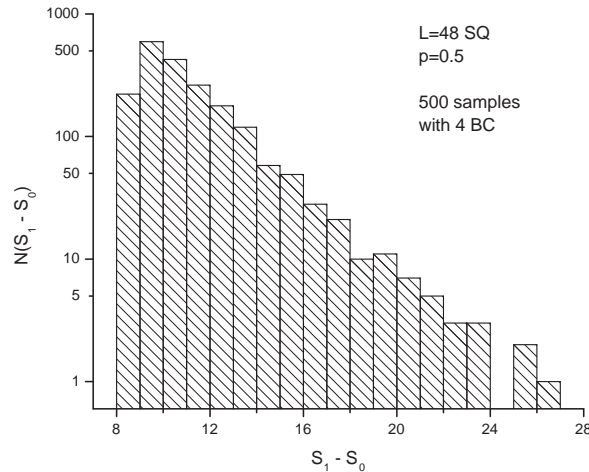


FIG. 4: Histogram of the distribution of  $S_1 - S_0$  for  $L = 48$ .

Stirling's approximation one sees immediately that the difference between using  $2\ln(L)$  and  $\ln(\ln((L^2)!))$  is a logarithmic correction to scaling. This logarithmic correction appears to be present in the data, however, and a much better fit is obtained if one does things as shown here.

If one uses  $2\ln(L - 3)$  an excellent fit over the range of the data is obtained. However, this seems completely artificial to the author. In any case the value of  $\rho = 0.1948 \pm 0.0008$  which one finds from this form is close to the one shown in Fig. 3. (The reason why the statistical error in this number is so small is that no contribution from the uncertainty in the fitting parameter “3” is included.)

The reason for taking the configuration average of  $\ln(S_1 - S_0)$  rather than taking the logarithm of  $\text{av}(S_1 - S_0)$  is that in this way we find the most probable value.<sup>20,21</sup> The probability distributions for  $S_1 - S_0$  are highly skewed, and the most probable value scales differently with  $L$  than  $\text{av}(S_1 - S_0)$  does. To illustrate this point, in Fig. 4 we show a histogram of the distribution of  $S_1 - S_0$  for the  $L = 48$  lattices. If one plots the data using  $\text{av}(S_1 - S_0)$ , one finds an apparent value for  $\rho$  of 0.233(3). Using the median value gives 0.222(3). It is the typical or most probable value which is the experimentally observable quantity, as established by Edwards and Anderson<sup>2</sup> for the spin glass.

From this analysis, we obtain the typical value of  $S_1 - S_0$  to be

$$S_1 - S_0 = f(L) \approx A[\ln((L^2)!)]^\rho, \quad (7)$$

with  $A = 1.696 \pm 0.019$ , or, using Stirling's approximation,

$$f(L) \approx A[L^2(2 \ln(L) - 1)]^\rho. \quad (8)$$

It follows immediately that the scaling of  $S_1 - S_0$  with  $L$  is approximately a power law, with an exponent close to 0.4, times  $\ln(L)$ . This variation with  $L$  is much more rapid than the hypothesis of Wang and Swendsen,<sup>19</sup> who argued for a dependence like  $4 \ln(L)$ . To this extent, it agrees with the claims of Jörg *et al.*<sup>11</sup>

To obtain the actual behavior of the low temperature specific heat, we must carry the analysis further. The heat capacity of a sample of size  $L \times L$  at temperature  $T$  is given by

$$C(L, T) = \langle (E(L) - \langle E(L) \rangle)^2 \rangle / T^2, \quad (9)$$

where the angle brackets indicate a thermal average, and we are using units in which Boltzmann's constant is 1.

Writing the partition function of a finite sample with periodic boundary conditions explicitly gives

$$Z(T) = \sum_{n=0}^{|E_0|/2} \exp(S_n - S_0 - 4n/T). \quad (10)$$

The heat capacity is then

$$C(L, T) = (T^2 Z)^{-1} \sum_{n=0}^{|E_0|/2} 16(n - n_*)^2 \exp(S_n - S_0 - 4n/T), \quad (11)$$

where  $n_*$  is the value of  $n$  for which the argument of the exponential has its maximum for a given sample at temperature  $T$ .

The average values of  $S_n - S_0$  for small values of  $n$  are shown in Fig. 5, over our full range of  $L$ . The slope defined by these points, omitting the  $n = 1$  points, is plotted versus  $1/L$  in Fig. 6. The limiting value of this slope for large  $L$  obtained from this plot is found to be

$$\psi = 0.842 \pm 0.003. \quad (12)$$

This means that for  $n \ll L^2$

$$S_n - S_0 \approx f(L)n^\psi, \quad (13)$$

and implies

$$(n_*(L, T))^{1-\psi} \approx \psi f(L)T/4. \quad (14)$$

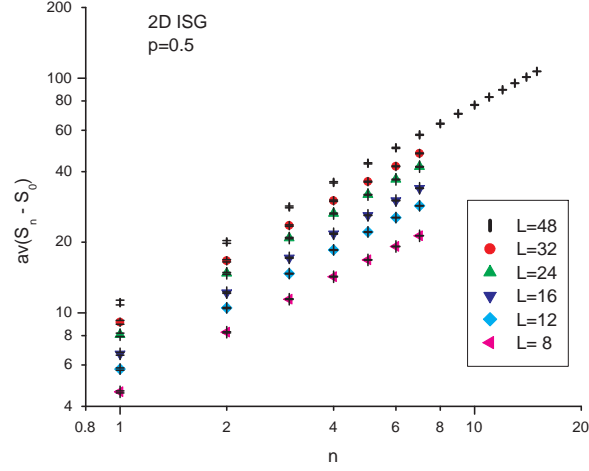


FIG. 5: (color online) Scaling of  $\text{av}(S_n - S_0)$  with  $L$ , for small values of  $n$ . The axes are scaled logarithmically.

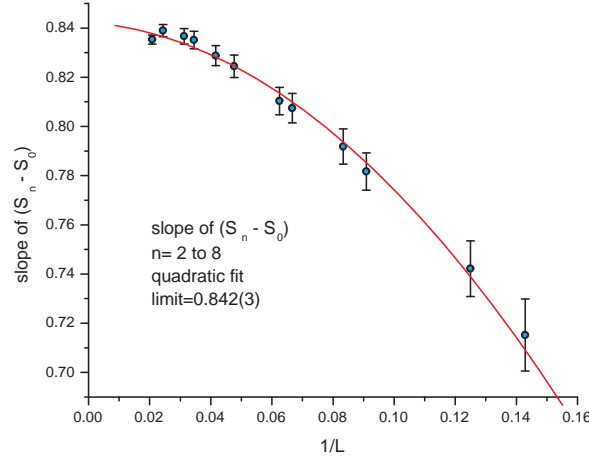


FIG. 6: (color online) Slope of  $\text{av}(S_n - S_0)$  vs.  $1/L$ , for  $n = 2$  to  $8$ .

This can only be valid, however, if  $0 < n_* \ll L^2$ . If we take the limit  $T \rightarrow 0$ , holding  $L$  fixed, then  $n_* \rightarrow 0$ . Thus the limiting low temperature behavior of  $C(L, T)$ , for any fixed  $L$  is proportional to  $\exp(-4/T)$ , as it must be. We expect to see this behavior when  $T < T_1$ , where

$$T_1(L) = 4[L^2(2\ln(L) - 1)]^{-\rho}/(\psi A) \quad (15)$$

is the temperature where  $n_* = 1$ . We have found a positive value for  $\rho$ , which means that



$T_1 \rightarrow 0$  as  $L \rightarrow \infty$ .

The reason for omitting the  $n = 1$  points shown in Fig. 5 from the fits is that they all lie well below the straight lines. The quantity  $S_1 - S_0$  does not behave in the same way that the other  $S_{n+1} - S_n$  do. The author understands this effect by analogy with the well-known behavior of random matrices. The gap at the band edge is special, because it only feels level repulsion from one side.

Substituting our expressions for  $n_*$  and  $S_n - S_0$  into Eqn. (10) gives

$$C(L, T) = 16T^{-2} \frac{\sum_{n=0}^{|E_0|/2} (n - (\psi AT/4)^{1/(1-\psi)} (L^2(2 \ln(L) - 1))^{\rho/(1-\psi)})^2 \exp(g(n, L))}{\sum_{n=0}^{|E_0|/2} \exp(g(n, L))}, \quad (16)$$

where

$$g(n, L) = n^\psi [A(L^2(2 \ln(L) - 1))^\rho - 4n^{1-\psi}/T]. \quad (17)$$

When we try to take the limit  $L \rightarrow \infty$  holding  $T$  fixed, we get a surprise. The exponent  $\rho/(1 - \psi)$  is  $1.216 \pm 0.033$ . Because this exponent is greater than 1, the power-law behavior described by the exponent of Eqn. (12) is only valid for  $T < T_x$ , where  $T_x$  must go to zero as  $L$  increases.  $n_*$  *cannot* become larger than  $L^2$ ! This condition requires that, when  $L \rightarrow \infty$ ,  $T_x$  must also go to zero at least as fast as

$$T_x(L) \sim 4L^{-2(\rho+\psi-1)}(2 \ln(L) - 1)^{-\rho}/(\psi A). \quad (18)$$

Although we do not have data to show that  $T_x$  actually behaves precisely in this way, it is at least plausible that  $T_x$  goes to zero more slowly than  $T_1$  as  $L$  increases, since  $\psi < 1$ .

What this means is that the singularity we are studying is subextensive, just as the thermal singularity above  $T_g$  is in the TAP mean-field theory.<sup>1,3</sup> It also means that for  $L$  large, but finite, we expect there exists a temperature regime  $T_1 \ll T \ll T_x$  in which the scaling behavior controlled by this singularity is observable.

$\rho$  controls the thermal behavior in the temperature range  $0 < T < T_1$ , and  $\psi$  controls the behavior in the range  $T_1 < T < T_x$ . Therefore, these exponents are independent. A simple scaling relation between exponents defined in different ranges of  $T$  which have independent behaviors is impossible. This statement is not in contradiction with the fact that the value of  $T_x$  clearly depends on both  $\rho$  and  $\psi$ . The entire procedure used here is quite similar to the theory of nested boundary layers.<sup>22</sup>

Since  $\langle E(L) \rangle$  is essentially  $4n_*(L, T)$ , the heat capacity for  $T_1 < T < T_x$  is easily seen to be proportional to  $T^{\psi/(1-\psi)}$ , which is  $T^{5.33 \pm 0.12}$ . Because  $T_x \rightarrow 0$  as  $L \rightarrow \infty$ , this behavior

disappears in the thermodynamic limit. The exponent  $2(\rho + \psi - 1)$  is  $0.068 \pm 0.009$ . This is small, so  $T_x$  is going to zero quite slowly. Thus the power-law behavior of  $C(L, T)$  should be visible for macroscopic values of  $L$ . Note that this effect is not caused by our choice of logarithmic averaging of  $S_1 - S_0$ , since the use of simple averaging would give a larger value for  $\rho$ .

Although our statistical errors are small, the estimate of  $\rho$  depends on our choice of the finite-size scaling fitting function. Notice that the estimate of the scaling exponent  $\alpha$  for the  $T$  dependence of  $C(L, T)$  depends only on  $\psi$ , and is independent of  $\rho$ . Therefore, our estimate

$$\alpha = -5.33 \pm 0.12 \quad (19)$$

is independent of whether  $T_x \rightarrow 0$  as  $L \rightarrow \infty$ .

All of the calculations for  $p = 0.5$  described above were repeated for  $p = 0.25$ . Using the same procedures as discussed above, we find for  $p = 0.25$  the exponents  $\rho = 0.1874 \pm 0.0019$  and  $\psi = 0.8527 \pm 0.0017$ . Therefore we obtain  $2(\rho + \psi - 1) = 0.080 \pm 0.007$  and  $\alpha = -5.79 \pm 0.08$ . These results are quite consistent with universality of the critical exponents, since the quoted statistical errors do not include any allowance for errors in the assumed scaling forms.

Recently, Jörg *et al.*<sup>11</sup> have claimed that a power-law behavior of  $C(L, T)$  is evidence that the QDE is in the same universality class as the CDE. However, they have not calculated  $\alpha$  directly. They have calculated the correlation length exponent  $\nu \approx 3.5$ , and assumed that  $\alpha$  could be obtained via the modified hyperscaling relation of Baker and Bonner.<sup>23</sup> The fact that our value of  $\alpha$  is not close to  $-7$  shows that this relation is not obeyed. Our value seems to indicate that the ordinary hyperscaling relation,  $d\nu = 2 - \alpha$ , is obeyed.  $\alpha$  has never been calculated directly for the CDE, so we cannot say whether the values of  $\alpha$  are the same for the QDE and the CDE.

Finally, we discuss the origin of the subextensive singularity. Such behavior in a 2D model probably requires the existence of some kind of long-range interactions. Such interactions are not present explicitly in our Hamiltonian, Eqn. (1), but they may arise spontaneously. Since domain walls are extended objects, it would not be very surprising for interactions between domain walls to have long range, especially at  $T = 0$ .

Using the same computer program which was used here to obtain the heat capacity and additional procedures described in a recent publication,<sup>6</sup> we have calculated the average

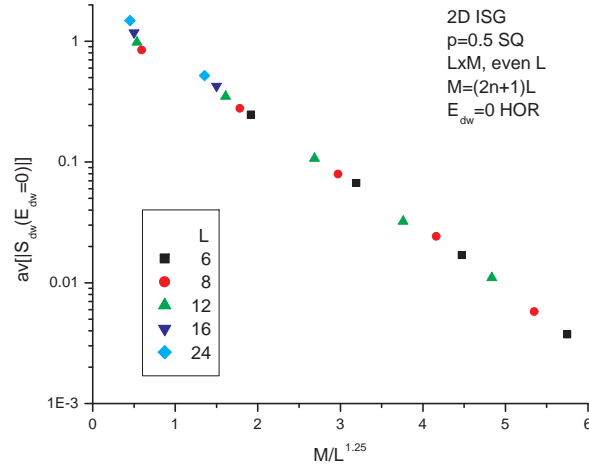


FIG. 7: (color online) Scaling of average entropy of zero-energy domain walls for lattices of size  $L \times M$  vs.  $M/L^{1.25}$ . These domain walls run across the lattice in the short direction, which has length  $L$ .

domain-wall entropy for zero-energy domain walls on lattices of size  $L \times M$ , where  $L \leq M$ . Remarkably, the average domain-wall entropy for the zero-energy domain walls which run across the lattice in the short ( $L$ ) direction scales to zero exponentially in the variable  $M/L^{1.25}$ . This is shown in Fig. 7. The exponent 1.25 is suggestive of the relation recently proposed by Amoruso, Hartmann, Hastings and Moore,<sup>24</sup> which gives a value of 1.25 for the fractal dimension of domain walls for this model. From the data displayed here we can say that this exponent must be  $1.25 \pm 0.05$ . Because their entropy scales to zero so rapidly, these zero-energy domain walls must be highly correlated.

This effect is strong evidence for long-range interactions between the zero-energy domain walls. It does not occur for domain walls of other energies. Amoruso *et al.* do not explicitly specify that the behavior of the zero-energy domain walls should be special. However, this was suggested by the work of Wang, Harrington and Preskill.<sup>25</sup> This domain-wall entropy calculation will be described more fully in a subsequent publication.<sup>26</sup>

In this work we have calculated in detail the low temperature thermal behavior of the 2D Ising spin glass with an equal mixture of  $+1$  and  $-1$  bonds. We have found that this behavior bears a strong qualitative resemblance to the behavior found in the TAP mean-field-theory analysis. For finite  $L$  there is a range of  $T$  for which  $C(L, T)$  is proportional to

$T^{5.33}$ . However, this behavior disappears slowly as  $L \rightarrow \infty$ . This subextensive behavior is attributed to correlations between zero-energy domain walls.

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